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Obtaining the *J*-integral by diffraction-based crack-field strain mapping

S.M. Barhli[a]*, L. Saucedo-Mora[b], C. Simpson[c,d], T. Becker[e], M. Mostafavi[f], P.J. Withers[c,d], T.J. Marrow[a]

[a]*Department of Materials, University of Oxford, Oxford, OX1 3PH, UK*
[b]*Institute Eduardo Torroja for Construction Sciences, s/ Serrano Galvache 4, Madrid, 28033, ES*
[c] *School of Materials, University of Manchester, Manchester, M13 9PL ,UK*
[d] *Research Complex at Harwell (RCaH), Harwell, Didcot, OX11 0FA ,UK*
[e]*Department of Mechanical and Mechatronic Engineering, Stellenbosch University, Stellenbosh, 7599, SA*
[f]*Department of Mechanical Engineering, University of Bristol, Bristol, BS8 1TR, UK*

Abstract

The analysis by diffraction of polycrystalline materials can determine the full tensor of the elastic strains within them. Point-by-point maps of elastic strain can thus be obtained in fine-grained engineering alloys, typically using synchrotron X-rays or neutrons. In this paper, a novel approach is presented to calculate the elastic strain energy release rate of a loaded crack from two-dimensional strain maps that are obtained by diffraction. The method is based on a Finite Element approach, which uses diffraction data to obtain the parameters required to calculate the J-integral via the contour integral method. The J integral is robust to uncertainties in the crack tip position and to poor definition of the field in the crack vicinity, and does not rely on theoretical assumptions of the field shape. A validation of the technique is presented using a synthetic dataset from a finite element model. Its experimental application is demonstrated in an analysis of a synchrotron X-ray diffraction strain map for a loaded fatigue crack in a bainitic steel.

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Keywords: *J*-integral; XRD; diffraction; EDXRD; Stress-Intensity Factor; strain mapping

1. Introduction

A recurrent fracture mechanics requirement is to quantify the field surrounding a crack that controls its

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propagation. With that aim, it is important to quantify the elastic strains around the crack, and various techniques exist that allow their point wise determination. In particular, the analysis of diffraction patterns, obtained with monochromatic X-ray diffraction (XRD), Energy-Dispersive polychromatic X-ray diffraction (EDXRD) or neutron diffraction (ND) can achieve this goal [[Allen, Hutchings (1985)], [Withers and Webster (2001)]], where a set of point measurements can be used to map the elastic strain field. Example applications include studies of fatigue crack overloads and closure [Lopez-Crespo, Mostafavi (Accepted for publishing)] [Allison (1979)], the role of residual strains in vicinity of the weld heat affected zones [Owen, Preston (2003)] and the mechanical shielding effect of crack bridging in stress corrosion cracking [Marrow, Steuwer (2006)]. Combined diffraction strain mapping and X-ray tomography [Steuwer, Edwards (2006)] has also been used to study the effect of overloads on fatigue cracks, and diffraction analysis of elastic strains can also be combined with strain measurement methods such as image and volume correlation [Marrow, Liu (2015)], allowing elastic strains to be separated from plastic strains and damage. To support such studies, it is useful to quantify the crack field, for instance the stress intensity factor of a fatigue crack has been obtained using a least-square field fit to elastic strain maps obtained by synchrotron X-ray diffraction [Belnoue, Jun (2010)].

The contour integral method based on the *J*-integral formulation is an alternative to field fitting methods, which have previously been applied to full-field displacement data to obtain stress intensity factors [Lopez-Crespo, Shterenlikht (2008)]. Independently developed by Cherepanov and Rice [[Cherepanov (1967)], [Rice (1968)]], the *J*-integral can be used to calculate the strain energy release rate directly from the displacement field around a crack, using knowledge of the stress-strain properties of the material. Its formulation is defined as a contour integral, which has zero value if no crack is present in the contour. Often implemented as a line integral, the *J*-integral can be rewritten as a surface or area integral using Green's theorem, and this formulation is convenient to implement in Finite Element (FE) analyses. One example of the direct evaluation of the *J*-integral from a measured crack displacement field is the JMAN method [Becker, Mostafavi (2012)]. The original JMAN Matlab code developed by Becker et al. takes as its input the full-field displacements from an image correlation analysis. It allows the user to define integration contours over which the J-integral is calculated, using the element-based virtual crack extension formulation [Parks (1977)].

A search of the literature finds no methods to determine the *J*-integral from strain-only datasets, such as those obtained by diffraction. However, there is a strong motivation to do this, as the *J*-integral method has some advantages over the field fitting methods. In particular, it is robust to uncertainties in the crack tip position and to poor definition of the field in the crack vicinity, and does not rely on theoretical assumptions of the field shape. In this work a method to determine the *J*-integral from elastic strain-only datasets is presented and benchmarked on a finite element dataset. The technique is then demonstrated on synchrotron EDXRD elastic strain maps around a crack tip in a bainitic steel compact tension (CT) specimen.

2. Materials and Methods

2.1. Numerical approach

The finite element formulation of the *J*-integral for a crack lying on the *x* axis is formalized by Equation 1, where σ_{ij} represents the 2-D stress tensor components; U_i the displacement components; W represents the strain energy density that for linear isotropic materials can be defined as $\frac{1}{2}\sum_{ij}\sigma_{ij}\varepsilon_{ij}$; and q is the virtual crack extension function whose value is 1 inside the inner integration contour and 0 outside the outer integration contours and is differentiable at all its points. The last term of the equation, A_{el}, expresses the element area.

$$J = \sum_{elements}\left[\left(\sigma_{xx}\frac{dUx}{dx} + \sigma_{xy}\frac{dUy}{dx} - W\right)\frac{dq}{dx} + \left(\sigma_{xy}\frac{dUx}{dx} + \sigma_{yy}\frac{dUy}{dx}\right)\frac{dq}{dy}\right] * A_{el} \quad (1)$$

The full 2-D elastic strain tensor can be obtained from an adequate treatment of diffraction data [Korsunsky, Wells (1998)], but not all the terms required in Equation 1 can be determined from these strains. In particular, dUy/dx cannot be directly extracted from the shear strain, as $\varepsilon_{xy} = dUy/dx + dUx/dy$. All other values are either determined directly from the strain measurement technique or can be calculated using the elastic modulus. To

address this missing value problem, the *Uy* displacement field must be obtained from the measured elastic strains, and then differentiated with respect to *x*. Integration of the strains in order to obtain the displacements was judged too complex, as the strain fields include a discontinuity (i.e. the crack), so a finite element approach has been applied.

The elastic strain map obtained by diffraction can be considered as equivalent to the elastic strains of a mesh of square quadrilateral elements where each element is centred on the measured ε_{xx}, ε_{yy} and ε_{xy} values. The mesh elements, which can be defined as plane strain or plane stress, have reduced integration formulation; this means that the elements only have one integration point (i.e. Gauss point) that is established at each element's centre. In a conventional FE simulation, the elastic strains at the integration points are computed using the displacements of the element nodes. In the analysis developed here, the compatibility conditions for linear elastic materials are used to solve the displacement field from the input strain field. Thus, the diffraction-measured elastic strains are used to find the originating displacement field, which is required to obtain the *J*-integral.

Consider the case of a diffraction-measured elastic strain map that is represented by a FE mesh of N×N quadrilateral 4-node elements; for each element a set of 3 equations can be defined that links the element node displacements to strains (one for each strain component), and this gives a total of $3N^2$ equations. There are 2 unknown orthogonal displacement values per node, so the total number of unknowns in the problem is $2(N+1)^2$. Therefore, any model with more than 5×5 elements will be over-constrained[1] and so can be solved and optimized to obtain the displacement field from the strain values. It is important to note that the elements next to the crack path are excluded from the analysis in order to avoid defining mesh connectivity where it is inappropriate.

A Matlab implementation of this approach has been created[2], it uses a matrix formulation such that $M \times X = B$ where B contains the elements' strain values, X contains the elements' node displacements and M ensures the correct definition of the equations (Fig. 1). The elements next to the crack path do not appear in the matrix equation; if a node is shared by four excluded elements, no displacement values will be calculated at this node. The size of the three matrices are respectively $(3N^2;1)$, $(2(N+1)^2;1)$, and $(3N^2;2(N+1)^2)$.

$$\begin{bmatrix} & & \\ & M & \\ & & \end{bmatrix} \begin{bmatrix} u_{x1} \\ u_{y1} \\ u_{x2} \\ u_{y2} \\ u_{x3} \\ u_{y3} \\ \dots \end{bmatrix} = \begin{bmatrix} \varepsilon_{xx1} \\ \varepsilon_{yy1} \\ \varepsilon_{xy1} \\ \varepsilon_{xx2} \\ \varepsilon_{yy2} \\ \varepsilon_{xy2} \\ \dots \end{bmatrix}$$

Fig. 1. Matrix formulation of the problem

A linear least-square solver with a "trust-region-reflective" algorithm [Coleman and Yuying (1996)] that is implemented natively in Matlab was chosen. By default the algorithm evaluates an approximate solution at each iteration via the method of preconditioned conjugate gradients (CG); in our case, the CG method was observed to induce noise in the results. It was replaced by a direct Cholesky factorisation method that is computationally more expensive, but was found to provide better quality results.

This method was incorporated within the JMAN Matlab code from Becker et al. [Becker, Mostafavi (2012)] to create JMAN_S (i.e. "*JMAN Strain*"). The developed code allows one to use the elastic strain field from a

[1] The problem can be considered over-constrained when the number of equations is larger than the number of unknowns. In this case this occurs for $3N^2 > 2(N+1)^2$, i.e. N>5.

[2] The Matlab code is available from the corresponding author.

diffraction experiment, without any displacement data, as an input to calculate the *J*-integral for a crack. In the calculation of the *J*-integral, stresses are obtained directly from the strains, using the crystal elastic modulus specific to the crystal planes of the diffraction analysis. The dUy/dx term is obtained from the solved displacement field, and elastic strains are obtained from the diffraction data. This is acceptable when the material's bulk elastic modulus is close to the elastic modulus of the diffracting crystal planes. A future implementation of the code will consider the cases where the crystal and bulk elastic moduli differ.

In the case where the experimental procedure does not provides a strain map on a regular grid, an interpolation step may be used to format the data correctly. A future development of the JMAN_S method may accept non-rectangular elements, so that irregular maps could be analysed without an interpolation step. In the current form, square elements of uniform dimension are used.

2.2. Benchmark and experimental dataset

To benchmark the method, a 2D finite element model of a pure mode I horizontal edge crack in a plate was created in the Abaqus FE software. Bi-linear, four-node, plane stress [3] quadrilateral elements with reduced integration were used with a linear elastic material model with moduli representative of an austenitic stainless steel (E=190 GPa, ν=0.3). Each element was a square of 0.6 × 0.6 mm. The resulting elastic strain field was used as an input for JMAN_S. An area of 50 × 50 mm around the crack tip was considered, with the sampling points lying on a regular grid of step size 0.6 mm. No interpolation was used as the FE results were already defined on a regular grid. The accuracy of the method was evaluated by comparing the obtained elastic strain energy release rate with that calculated directly by the original FE solution.

The experimental application was realized using EDXRD elastic strain maps that had been obtained for a 5×5 mm region centred on a fatigue crack tip of a bainitic steel Compact Tension specimen (W=50 mm and a/W = 0.45 as defined in ASTM standard geometry [ASTM (2003)]); the fatigue crack was introduced prior to the experiment using standard load shedding, to a maximum stress intensity factor 10.5 MPa $m^{0.5}$. The data were obtained at the I12-JEEP (Joint Engineering, Environmental, and Processing) beamline at the UK Diamond Light Source as part of experiment EE12205. A 100 kN servo-hydraulic Instron machine was used to load the specimen in situ in the X-ray beam. The specimen thickness was 10 mm and each strain map was a combination of 2 scans: a fine scan, used next to the crack tip, with a gauge measurement volume of 50×50×4000 μm; and a coarser scan used in the wider area with a gauge measurement volume of 100×100×4000 μm. All the results were interpolated onto a regular square grid of step size 200 μm using a bi-linear interpolator. The diffracting gauge volume was at the specimen mid-thickness; a plane strain condition could therefore be assumed.

The {110} Bragg diffraction peak was used and treatment of data from the 23-elements EDXRD detector elements allowed the creation of ε_{xx}, ε_{yy} and ε_{xy} maps using the pyXe python package[4]. The coordinate system is defined in Fig. 4. Data were obtained at 4 load levels to apply increasing stress intensity factors (SIF), which were calculated using the standard analytical solution and surface crack length measurements.

3. Results and discussion

3.1. Benchmarking

The JMAN_S method was applied to the FE exported elastic strain field of the benchmark model. A mask of 2 elements width was applied on the crack path and extended 2 elements beyond the crack tip. The masked elements are excluded from the contour integral and the displacement solving step. This is necessary to define both the start and end of the integration contour, and the unconnected regions in the displacement field solution. Examination of

[3] The relation between displacements and in-plane strains in a 2D simulation is the same for plane strain and plane stress elements.
[4] PyXe is a software developed by Simpson, C. (2016). DOI. 10.5281/zenodo.50185

the displacement field that is obtained from the strains shows that the code quite accurately retrieved the original displacement values from the strain data. The example in Fig. 2 shows the *Uy* displacement, which is the most significant displacement for a crack parallel to the *x*-axis.

The FE displacements have been corrected for rigid body movement, so the displacement at the crack tip is zero. The negative solved displacements match the original FE displacements, whereas the positive displacements have the same gradient, but with the solved values decreased slightly by 80 µm (Fig. 2b). This is likely to be due to the errors in the solved displacements that have the same y-coordinate as the crack tip (Fig. 2a), and this error propagates through the displacement field. It has a negligible effect on the displacement gradient field. The *J*-integral was evaluated using JMAN_S and in the original FE model on multiple contours to check for path independency; the outer contours were centred on the crack tip and extended radially in all directions, the inner contour had a fixed size of 4 x 4 mm, also centred on the crack tip. The JMAN_S *J*-integral converged (Fig. 3) within 4 contours with less than 0.5% relative error. The convergence of the original FE model within 2 contours is shown for comparison.

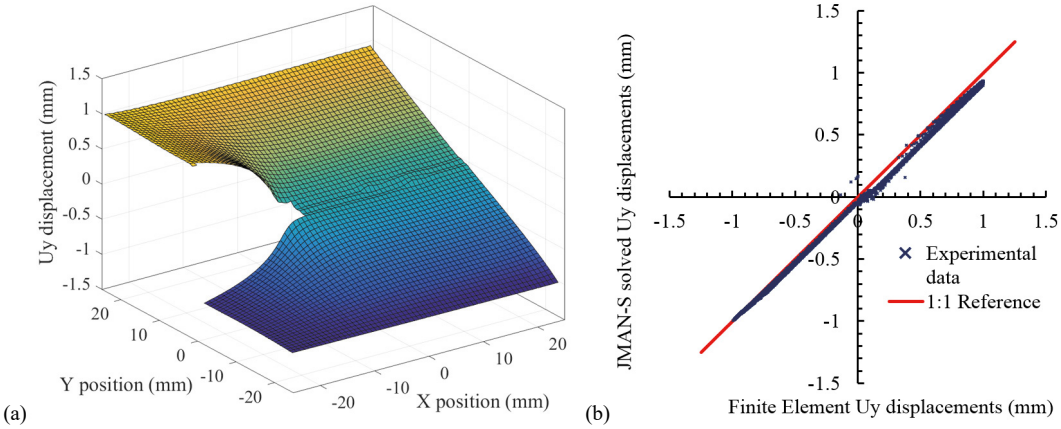

Fig. 2. (a) Uy displacement field solved from FE strain data (b) Original FE displacements versus JMAN_S displacements, the line corresponds to a 1 to 1 relationship

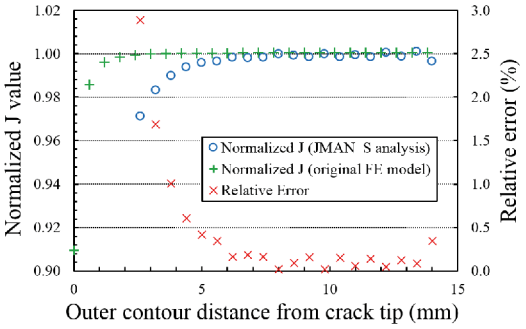

Fig. 3. J-integral calculation from FE strain dataset using JMAN_S and original FE data

3.2. Experimental

Examples of the experimental data, obtained at an applied stress intensity factor of 30 MPa.m$^{0.5}$, are shown in Fig. 4. In the application of the JMAN_S method, the calculated *J*-integral converged in all cases and was contour independent (Fig. 5a). The {110} specific modulus of 210 GPa [Hutchings, Withers (2005)] was used in the

computation of the stresses; the bulk tensile elastic modulus for bainitic steel is between 205-210 GPa. The results are summarised in Fig. 5b, in comparison with the applied stress intensity values. For comparison, the *J*-integral values have been converted to stress intensity factors using Equation 2, which is valid for plane strain condition, where the tensile elastic modulus is 210 GPa and Poisson's ratio is 0.3.

$$K_I = \sqrt{J\left(\frac{E}{1-\nu^2}\right)} \qquad (2)$$

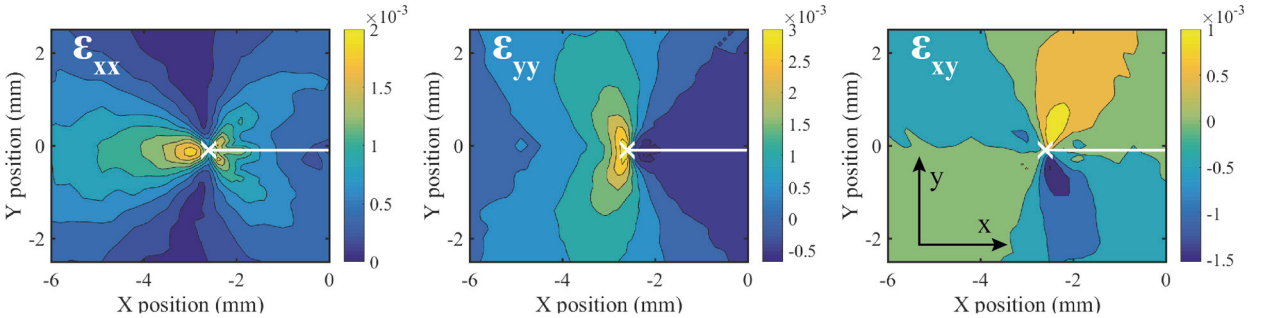

Fig. 4. EDXRD strain maps for an applied K value of 30 MPa.m$^{0.5}$. The crack tip and crack path are shown in white.

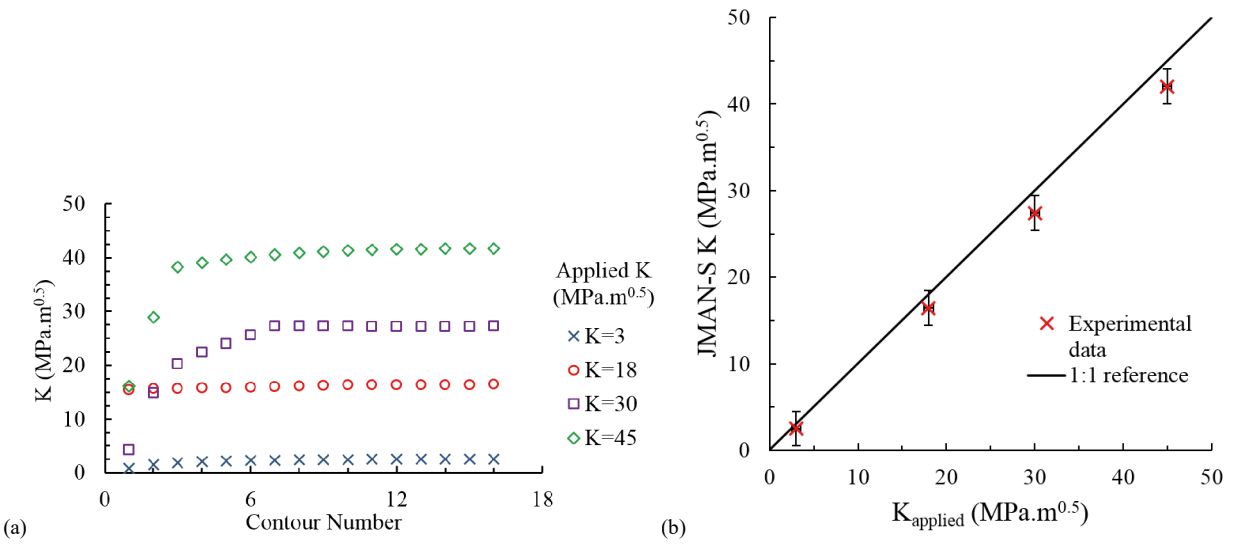

Fig. 5. (a) J-integral contour independence and convergence at different applied stress intensity factors, the outer contour distance to crack tip increase linearly with each contour (b) Comparison of the applied stress intensity factor, $K_{applied}$, with JMAN_S calculated values

The SIF values determined with the JMAN_S method show good agreement with the applied stress intensity factors. The uncertainty in the applied value, mostly due to crack length determination errors, is estimated to be less than ±0.5 MPa m$^{0.5}$. The random error in the stress intensity factor obtained via JMAN_S is taken as the standard deviation over the last 10 contours, and is less than 2 MPa m$^{0.5}$ in all cases. There is a systematic difference between the applied and calculated stress intensity factors. This may be due to extrinsic effects such as alignment errors in the loading of the crack, or the difference between the bulk and crystal elastic behaviour, and is the subject of further investigation and calibration studies. Nonetheless, the agreement between the expected and measured stress intensity factors is good.

The JMAN-S method requires a correctly solved displacement field to be obtained from the measured elastic strain data, but experimental noise may cause the solver to converge on erroneous solutions (local minima). This

can be tested for since the resulting displacement field, in the case where a local minimum is found, is clearly wrong; an incorrectly solved field exhibits oscillating and abnormally high values of displacement and is not consistent with the well-known form of displacement field for a crack. The mask dimensions may then be adjusted to censor poor data in the vicinity of the crack until a satisfactory convergence is obtained - a change of one element size is usually sufficient. An automated iterative approach to mask dimension optimization is currently used. For a given mask, the solved displacement field is tested against a William series fit; a quality grade is determined as the square sum of residuals, normalized by the maximum displacement value and non-masked area.

4. Conclusion

A novel technique is presented to characterize the crack driving force of a loaded crack, as a *J*-integral elastic strain energy release rate, from diffraction-measured 2-D elastic strain datasets. In principle, it can be used with any experimental method that retrieves the full 2-D elastic strain tensor. The critical step is the solution of the equivalent displacement field, using a finite element approach and the compatibility conditions in linear elastic mechanics.

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